UNIVERSITY OF CALIFORNIA BERKELEY
Department of Civil Engineering
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Structural Engineering,
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HW 5: Due October 29

Equilibrium Lattice Configurations, Deformation Gradients, Phonon-Dispersion Curves

For this assignment you will complete a phonon dispersion curve program that has been partially written for you. In particular, we have provided you with a set of utility functions which you can then incorporate into your program. The function names and their input/output format are given below. The last two functions are incomplete and hence should be written so that you can use the full code to get the required equilibrium lattice configurations and phonon-dispersion curves. A ZIP file of the routines is included with this assignment.

MATLAB Phonon Program Headers

1. `[energy, force, stiffness] = morse(V0,a0,r0,r)`
   Returns the function value (`energy`), the first derivative (`force`) and the second derivative (`stiffness`) of the Morse potential with parameters `V0, a0, r0` at function value `r`.

2. `[a,b,c,alpha,beta,gamma] = get_cell_3D(a1,a2,a3)`
   Calculates the six lattice parameters from the three (column) lattice vectors.

3. `[a1,a2,a3] = get_lattice_vec_3D(a,b,c,alpha,beta,gamma)`
   Inverse of the previous function.

4. `out_basis_3D(bv)`
   Prints basis vectors that are stored as columns of a `3 x s` matrix `bv`, where `s` is the number of basis vectors (and thus the number of atoms per unit cell).

5. `out_cell_3D(a,b,c,alpha,beta,gamma)`
   Prints lattice parameters.

6. `out_lattice_3D(a1,a2,a3)`
   Prints lattice vectors.

7. `plot_lattice_3D(a1,a2,a3,bv,m,name)`
   Plots the lattice with (column) lattice vectors `a1, a2` and `a3` and the `3 x s` matrix `bv` formed by the column basis vectors where the `1 x s` mass vector `m` is used to scale the atom representations relative to each other. The string name contains the name to be displayed as header of the figure. To plot deformed lattices, pass in `F*a1, F*a2` and `F*a3` and the corresponding energy-minimizing `bv` where `F` is the deformation gradient. This routine plots a $4 \times 4 \times 4$ part of the superlattice.

8. `[energy]=lattice_energy_3D(a1,a2,a3,bv,F,V0,a0,r0,N)`
   Returns the energy per unit super cell of a lattice described by lattice vectors `a1, a2` and `a3` and the `3 x s` matrix `bv` formed by the column basis vectors, stretched by deformation gradient `F`, with interactions described by the `s x s` matrices `V0, r0` and `a0` using a parallelepiped super cell with `N` unit cells in each direction. To calculate the energy of the reference configuration, simply chose $\mathbf{F} = \mathbf{I}$.

9. `[a1,a2,a3,bv] = equil_lattice_3D(a1,a2,a3,bv,V0,a0,r0,N)`
   Returns (column) lattice vectors `a1, a2` and `a3` and the `3 x s` matrix `bv` formed by the column basis vectors of the closest local minimum energy configuration to the supplied guess given the `s x s` interaction matrices `V0, r0` and `a0` using a parallelepiped super cell with `N` unit cells in each direction.

10. `[bv] = affine_equil_lattice_3D(a1,a2,a3,bv,F,V0,a0,r0,N)`
    Returns the `3 x s` matrix `bv` formed by the column basis vectors minimized for a deformation of the reference lattice given by lattice vectors `a1, a2` and `a3` with deformation gradient `F` whose interactions are described by interaction matrices `V0, r0` and `a0` and for which a parallelepiped super cell with `N` unit cells in each direction is used.

INCOMPLETE FUNCTIONS

11. `[Dmat,M]=dynam_3D(a1,a2,a3,bv,F,V0,a0,r0,m,k,N)`
    Returns the `3s x 3s` dynamic matrix `Dmat` and the `3s x 3s` mass matrix `M` for a given wave vector `k` and a lattice described by (column, reference) lattice vectors `a1, a2, a3` and the `3 x s` matrix (minimized!) column basis vectors `bv` when stretched by the corresponding deformation gradient `F`. Here `V0, r0` and `a0` are the interaction matrices, `m` is the `1 x s` mass vector and `N` is the number of unit cells in each direction.

12. `phonon_2lattice_3D`
    Main file giving the structure of the problem.

Problem Definition : Dispersion in a 3-dimensional 3-basis lattice

A 3-dimensional lattice consists of 3 basis atoms whose masses are given as $m_1 = 44$ amu, $m_2 = 30$ amu and $m_3 = 50$ amu. The interaction between the different basis atoms is governed by two-body Morse potentials given by

$$V(r) = V_0\Big(e^{-2a_0(\frac{r}{r_0}-1)} - 2e^{-a_0(\frac{r}{r_0}-1)}\Big), \tag{1}$$

where r is the interatomic distance between two atoms and V_0, a_0 and r_0 are parameters that depend on the interacting atoms. These interaction parameters are given as

$$r_0 = \begin{bmatrix} 3.2 & 1.5 & 1.8 \\ 1.5 & 3.2 & 1.9 \\ 1.8 & 1.9 & 3.2 \end{bmatrix} \text{ Å}, V_0 = \begin{bmatrix} 3.0 & 0.3 & 0.4 \\ 0.3 & 3.0 & 0.5 \\ 0.4 & 0.5 & 3.0 \end{bmatrix} \text{ eV, and } a_0 = \begin{bmatrix} 3.2 & 1.2 & 1.3 \\ 1.2 & 3.2 & 1.4 \\ 1.3 & 1.4 & 3.2 \end{bmatrix},$$

where $r_{0_{ij}}$, $V_{0_{ij}}$ and $a_{0_{ij}}$ are the values for the interaction parameters between basis atoms of type i and j. The lattice is paramatrized by six parameters (three lengths a, b, c and three angles

α, β, γ where α is the angle between the lattice vectors $\boldsymbol{a}_2$ and $\boldsymbol{a}_2$, β is the angle between the lattice vectors $\boldsymbol{a}_3$ and $\boldsymbol{a}_1$, and γ is the angle between the lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$). The three lattice vectors are related to these six parameters by

$$\boldsymbol{a}_1 = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \qquad \boldsymbol{a}_2 = \begin{pmatrix} b\cos(\gamma) \\ b\sin(\gamma) \\ 0 \end{pmatrix}, \tag{2}$$

and $\boldsymbol{a}_3$ can be obtained from

$$\boldsymbol{a}_1 \cdot \boldsymbol{a}_3 = ac\cos(\beta), \qquad \boldsymbol{a}_2 \cdot \boldsymbol{a}_3 = bc\cos(\alpha), \qquad \boldsymbol{a}_3 \cdot \boldsymbol{a}_3 = c^2\,. \tag{3}$$

As discussed in class, the shifts of basis atoms 1, 2 and 3 in each unit cell with respect to the lattice is described using vectors $\hat{\boldsymbol{b}}_1$, $\hat{\boldsymbol{b}}_2$ and $\hat{\boldsymbol{b}}_3$[1]. Without loss of generality, choose $\hat{\boldsymbol{b}}_1 = \boldsymbol{0}$ and keep it fixed during all calculations.

1. Equilibrate the (unstretched , *i. e.*, $\mathbf{F} = \mathbf{I}$) lattice by minimizing its (0K) potential energy with lattice parameters and the shift using the starting guess as

$$a = 2.21\text{Å}, \qquad b = 2.21\text{Å}, \qquad c = 2.21\text{Å} \tag{4}$$

$$\alpha = 60^\circ, \qquad \beta = 120.4^\circ, \qquad \gamma = 120^\circ\,. \tag{5}$$

   The basis vectors are located at

$$\hat{\boldsymbol{b}}_1 \sim \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \hat{\boldsymbol{b}}_2 \sim \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}, \qquad \hat{\boldsymbol{b}}_3 \sim \begin{pmatrix} 0.2 \\ 0.3 \\ 0.0 \end{pmatrix}. \tag{6}$$

   Plot the resulting structure, print its lattice and basis vectors and calculate its potential energy.

2. Write the function that calculates the dynamical matrix $\boldsymbol{D}$ and the corresponding matrix $\boldsymbol{M}$ using N = 11[2] (*i.e.*, five neighbors in each direction). Do not assume nearest neighbor interactions. Sum over the whole supercell.

3. Determine all allowable wave vectors $\boldsymbol{k}$ that are parallel to the reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ and $\boldsymbol{b}_3$. Along each, direction, calculate the corresponding frequencies $\omega(\boldsymbol{k})$ and plot on a single graph.[3]

4. Subject the lattice to a homogeneous deformation described by

$$\boldsymbol{F} = \begin{bmatrix} 1 & 0.5 & 0 \\ 0 & 1.2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{7}$$

   and calculate the corresponding equilibrium lattice structure by minimizing with respect to the basis vector $\hat{\boldsymbol{b}}_2$ and $\hat{\boldsymbol{b}}_3$ by choosing $\hat{\boldsymbol{b}}_1 = (0; 0; 0)$. Plot the resulting configuration, print the corresponding lattice and basis vectors and calculate its potential energy.

[1] To distinguish the basis atom vector from the reciprocal lattice vectors, we will decorate them with a hat.
[2] N must be odd for the given routines to work!
[3] $\boldsymbol{f}$ was used in lecture for the wave vector but here we use $\boldsymbol{k}$ as it is more standard.

5. Calculate the dynamical matrix $\boldsymbol{D}$ and the mass matrix $\boldsymbol{M}$ for the stretched lattice using N = 11. Determine the allowable wave vectors $\boldsymbol{k}$ that are parallel to the reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ and $\boldsymbol{b}_3$. For each direction, calculate and plot the corresponding frequencies $\omega(\boldsymbol{k})$ on a single graph, *i.e.*, plot the dispersion curves.

To solve this problem, you may use any of the functions in the phonon.zip file from bspace. Your main efforts will involve writing the `dynam_3D.m` and `phonon_2lattice_3D.m` files as they are incomplete. The function names and their explanations are given at the start of the assignment.